# **ENDF/B-VIII.0**

D. Brown for the Cross Section Evaluation Working Group



a passion for discovery



### ENDF/B-VIII.0 was released on 2 Feb. 2018 by the Cross Section Evaluation Working Group (CSEWG)



### Integrates contributions for many sources

- Neutron Standards IAEA, NIST
- CIELO Pilot Project BNL led Fe, LANL led <sup>16</sup>O and <sup>239</sup>Pu, IAEA led <sup>235,238</sup>U
- Many new and improved neutron evaluations (DP, Crit. Safety, NE, USNDP)
- New thermal scattering libraries (Crit. Safety, Naval Reactors)
- Charged particles USNDP (LLNL)
- New atomic data (LLNL)
- Success rests on EXFOR library

  IAEA project but USNDP (BNL) coordinates

  compilation of reaction data for Western Hemisphere

Happy
50 th
Anniversary!\*

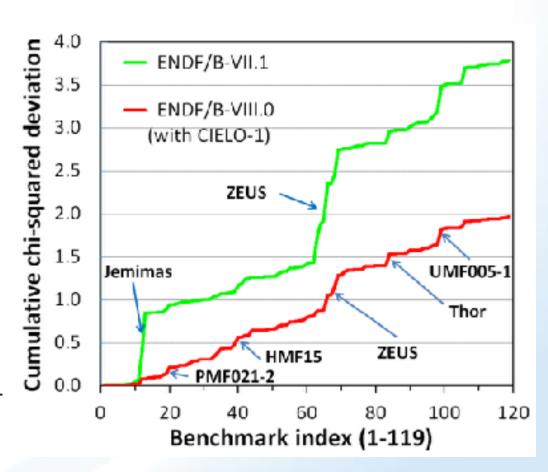




# ENDF/B-VIII.0 is our best performing and highest quality library yet



- Validate by simulating well characterized systems
  - 1198 critical assembly benchmarks
  - 14 MeV & <sup>252</sup>Cf(sf) source transmission
  - Many other tests
- Quality also assured by
  - ADVANCE continuous integration system at BNL
  - Annual Hackathons



M.B. Chadwick et al, Nuclear Data Sheets 148, 189 (2018)



# Library and evaluations detailed in Nuclear Data Sheets vol. 148 (2018)



- ENDF/B-VIII.0: D. Brown et al., Nuclear Data Sheets 418, 1 (2018)
- Neutron Data Standards: A. Carlson et al.,
   Nuclear Data Sheets 418, 143 (2018)
- CIELO Overview: M.B. Chadwick, et al.,
   Nuclear Data Sheets 148, 189 (2018)
- CIELO Iron: M. Herman, et al.,
   Nuclear Data Sheets 148, 214 (2018)
- CIELO Uranium: R. Capote, et al.,
   Nuclear Data Sheets 148, 254 (2018)
- **PFNS evaluation**: D. Neudecker, *et al.*, Nuclear Data Sheets 148, 293 (2018)
- <sup>239</sup>Pu(n,g) measurement: S. Mosby, et al.,
   Nuclear Data Sheets 148, 312 (2018)
- <sup>235</sup>U PFNS measurement: M. Devlin, et al., Nuclear Data Sheets 148, 322 (2018)



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#### Special Issue on Nuclear Reaction Data

Special Issue Editor: Povel Obložneký Special Issue Assistan: Editor: Bosis Pritychenko

#### Centents

A.D. Carlson, V.G. Pomyurv, R. Capote, G.M. Bale, Z. P. Chen, L. Darun, F. J. Hambrich, S. Kunieda, W. Manniart, B. Marcindevicius, R.O. Nelson, D. Seudicker, G. Noguere, M. Parin, S. Simskov, P. Schillebeccke, D. L. Smith, K. Tao, A. Trkov, A. Wallher, W. Wang

Costenti continuedon the back cover page.



# Outline for remainder of talk



- We didn't "change anyone's answers"
- Big changes that "didn't change anyone's answers": <sup>235,238</sup>U, <sup>239</sup>Pu, and H<sub>2</sub>O
- Other important changes that "maybe changed answers": <sup>16</sup>O, <sup>nat</sup>C, Fe, graphite







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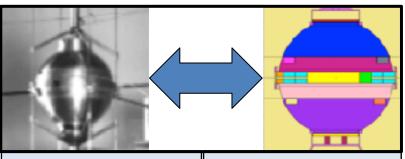
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Anniversary!\*





### There are many ways to "get the right answer"





BRC09 (CEA)  $k_{eff}$ =1.00082(11)

ENDF-VII.1  $k_{eff}$ =1.00060(12)

How does  $k_{eff}$  change when a BRC09 value is replaced by one from ENDF-VII.1?

Quantity	$\Delta k_{eff}$ (1000th's of %)		
Fission	-138		
Capture	+269		
Elastic Scattering	-638		
Inelastic Scattering	+522		

The end result is a lack of confidence in modeling systems that significantly differ from the integral benchmark

- E. Bauge, et al. (CEA-DAM)
- Swap portions of one evaluation for other until completely swapped
- Elastic & inelastic scattering provided biggest swing

Figure from L. Bernstein



# Situation "unchanged" in VIII.0



#### Pu-239 CEA-CIELO to LANL-CIELO

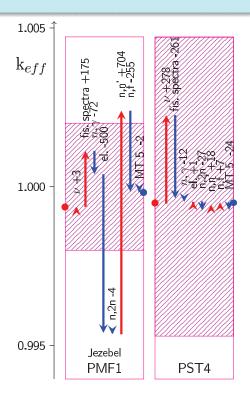


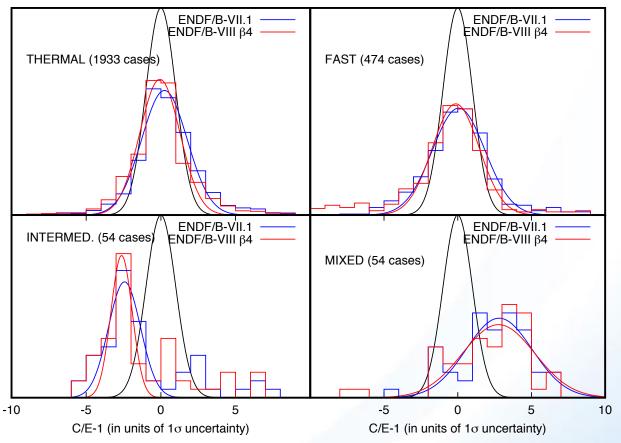
FIG. 28. (Color online) Simulations of criticality k-eff for <sup>239</sup>Pu for two critical assemblies: a fast assembly (Jezebel, PMF-1), and a thermal assembly (PST-4). This figure shows that both LANL CIELO-1 (ENDF/B-VIII.0) and CEA CIELO-2 (JEFF-3.3) predict similar k-eff values, but do so for very different reasons. The changes in criticality are evident when individual cross section channels are substituted between the two evaluations.



M. Chadwick et al., Nuclear Data Sheets 418, 189 (2018)

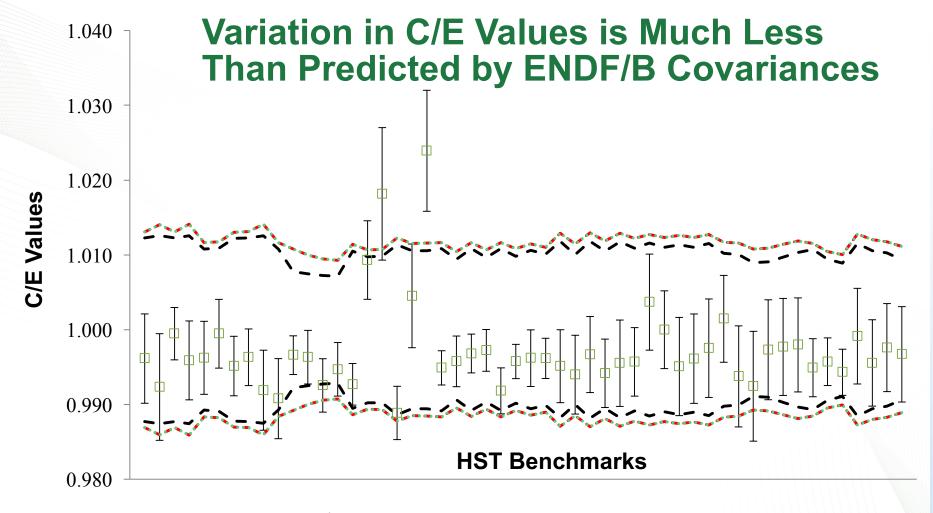
## We focused on thermal & fast applications





M. Chadwick et al., Nuclear Data Sheets 418, 189 (2018)

FIG. 29. (Color online) The distribution of C/E, in units of the combined benchmark and statistical uncertainty. The normal distribution (in black) would be the perfect situation.



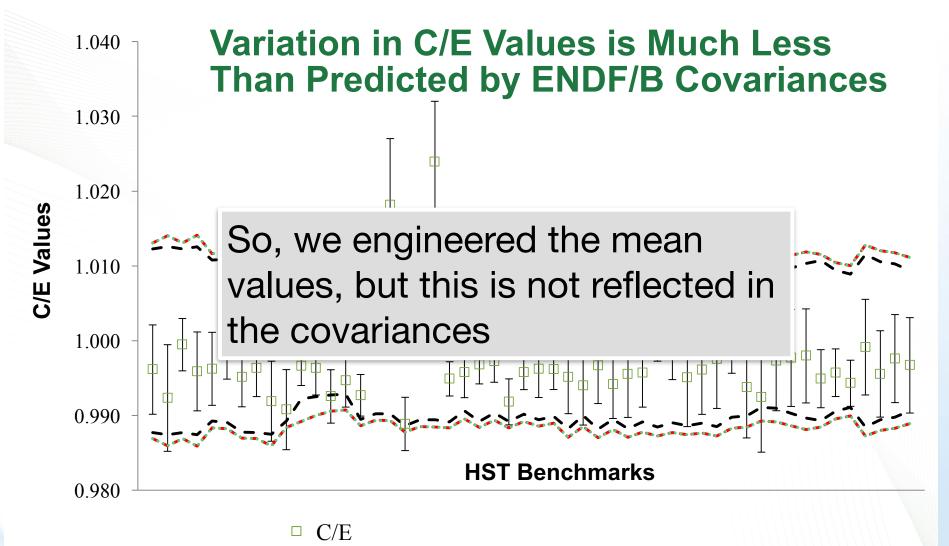
 $\Box$  C/E

- - SCALE 6.2 Covariance Library

--- ENDF/B-VIII Beta 5 Covariance Library

..... ENDF/B-VIII Beta 5 Covariance with SCALE 6.2

M. Williams, CSEWG meeting, Nov 2017



M. Williams, CSEWG meeting, Nov 2017

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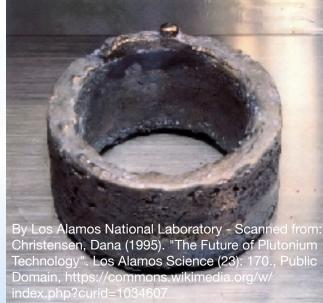


# Large overlap in evaluations of Big 3



- Neutron Data Standards: (n,f) cross section
- P(nu) for neutrons and gammas (Talou)
- Fission energy release (Lestone)
- PFNS & associated cov. (Neudecker)
- PFGS new, resolves long standing problem with fission gammas (Stetcu)
- Feedback from benchmarks
- Main differences: treatments of RR & Fast parts of evaluation

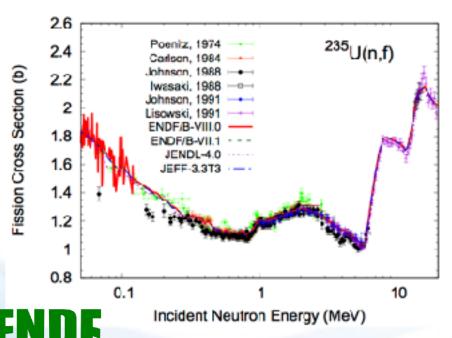


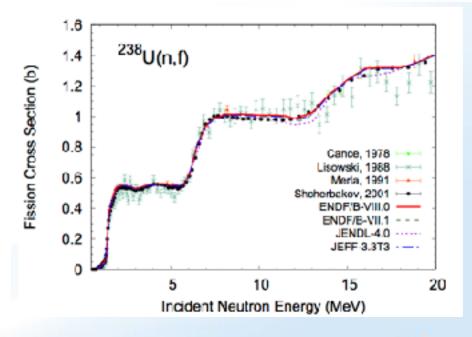


#### TABLE XXXII. Neutron Data Standards.

<b>Each major ENDF</b>
release is built off
the newest release
of the Neutron Data
Standards

Standards Energy Range
1 keV to 20 MeV
0.0253 eV to 50 keV
0.0253 eV to 1.0 MeV
0.0253 eV to 1 MeV
0.0253 eV to 1 MeV
10 eV to 1.8 MeV
0.0253 eV, 0.2 to 2.5 MeV, 30 keV MACS
0.0253 eV, 7.8-11 eV, 0.15 MeV to 200 MeV
2 MeV to 200 MeV
Prompt fission neutron spectra







D. Brown et al., Nuclear Data Sheets 418, 1 (2018)



# Unrecognized systematic uncertainty estimated and included



TABLE IX. Unrecognized systematic uncertainties from the analyses of the (weighted) standard deviations of the distributions for cross sections and  $\bar{\nu}_{tot}$  for  $^{252}$ Cf(sf). The  $\bar{\nu}_{tot}$  for  $^{252}$ Cf(sf) unrecognized systematic uncertainty was determined to be 0.4 %. All thermal neutron-induced  $\bar{\nu}_{tot}$  unrecognized systematic uncertainties are also assumed to be 0.4 %.

Cross section	Unrecognized systematic				
	uncertainty $(\%)$				
H(n,n) total	0.34				
$^6\mathrm{Li}(\mathrm{n,t})$	0.5				
$^{10}\mathrm{B}(\mathrm{n,}\alpha_1\gamma)$	0.8				
$^{10}\mathrm{B}(\mathrm{n,}\alpha)$	0.8				
C(n,n) total	0.65				
$\mathrm{Au}(\mathrm{n},\!\gamma)$	1.7				
$^{235}U(n,f)$	1.2				
$^{238}U(n,f)$	1.2				
$^{238}\mathrm{U}(\mathrm{n},\gamma)$	1.7  below  1  MeV				
$^{238}\mathrm{U}(\mathrm{n},\gamma)$	2.4 for 1 MeV and above				
<sup>239</sup> Pu(n,f)	1.2				

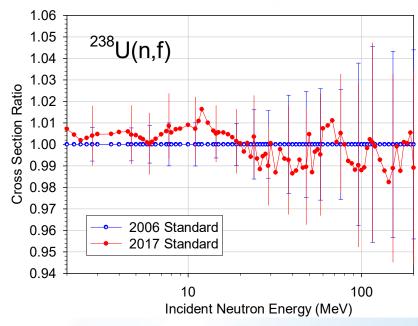
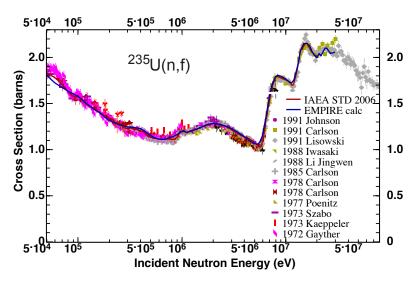


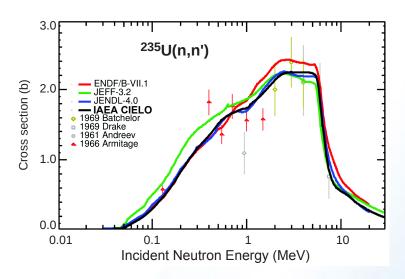
FIG. 14. (Color online) Comparison of the  $^{238}$ U(n,f) cross section from the 2017 evaluation with the 2006 standards evaluation. The unrecognized systematic uncertainty of 1.2 % has been included in the 2017 data. The baseline at 1.00 is the 2006 standards evaluation.

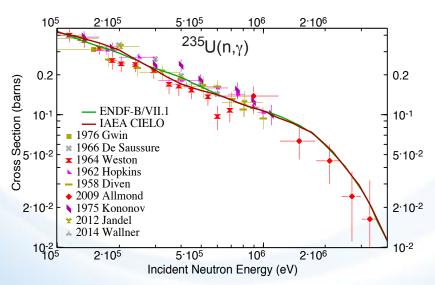


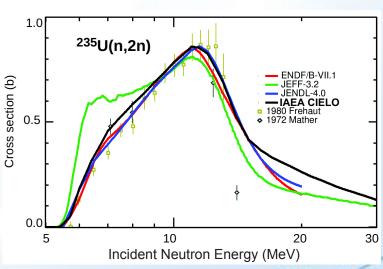
### Other cross sections adjusted to match fission











Brockhaven Science Associates (b) Fast neutron range above 100 keV.

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### Scattering data carefully reevaluated for <sup>238</sup>U



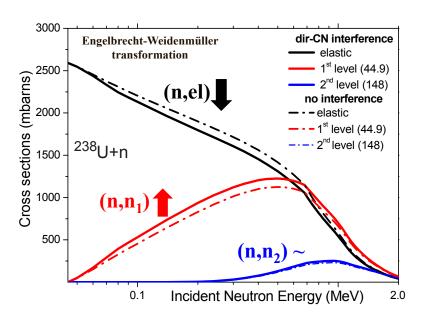


FIG. 17. (Color online) Neutron-induced reaction cross sections on  $^{238}$ U (top) and effect of the Engelbrecht-Weidenmüller transformation [179] on elastic and inelastic scattering on the first two excited levels of  $^{238}$ U (bottom). Experimental data in the top panel have been taken from EXFOR [91].

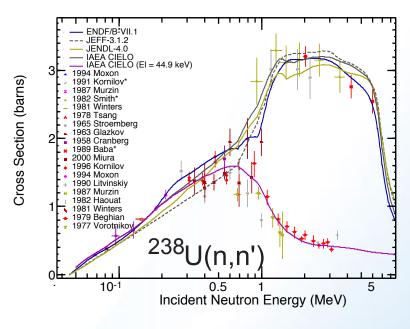


FIG. 18. (Color online) Calculated total and partial inelastic  $^{238}$ U(n,n') cross sections on 45 keV level compared with experimental and evaluated data files. Experimental data have been taken from EXFOR [91].

R. Capote et al., Nuclear Data Sheets 418, 254 (2018)

- Dispersive OMP tuned to major actinides
- Proper treatment of (in)elastic mixing though E-W transform
- Proper compound angular distributions
- (n,n'g) data WAS NOT used



### Scattering data carefully reevaluated for <sup>238</sup>U



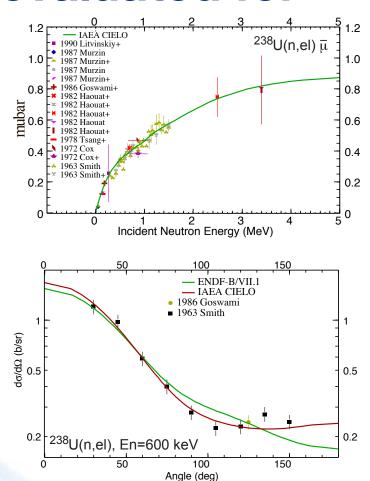
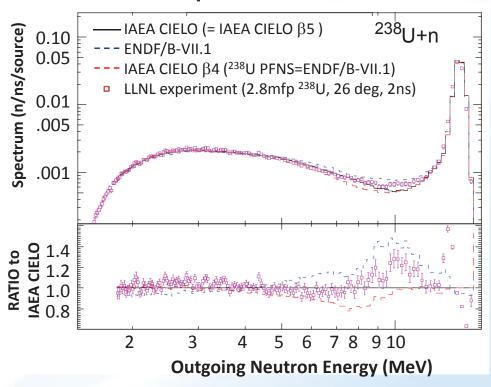


FIG. 19. (Color online) Average cosine of neutron elastic scattering  $\overline{\mu}$  on <sup>238</sup>U (top). Angular distribution of neutron elastic scattering at 650 keV incident energy (bottom) on <sup>238</sup>U. Experimental data have been taken from EXFOR [91].

# Excellent performance in Pulsed Sphere test



R. Capote et al., Nuclear Data Sheets 418, 254 (2018)

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### Main Updates from ENDF/B-VII.1



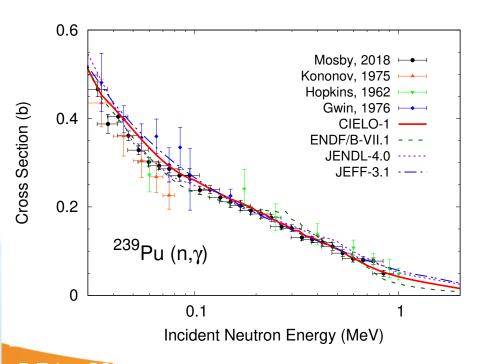
- Resonance region
  - Adoption of WPEC SG-34 results up to 2.5 keV
  - New resonance parameters and nubar values
- Fast region: not a new full-blown evaluation!
  - Capture
    - Experimental data by Mosby et al. (DANCE, LANL)
    - Theoretical advances (Kawano)
  - Fission
    - Adoption of new IAEA standards result
  - Prompt Fission Neutron Spectrum
    - Chi-nu data (cf. Kelly's talk) still preliminary
    - New evaluation above 5 MeV incident neutron energy
  - Updated covariances

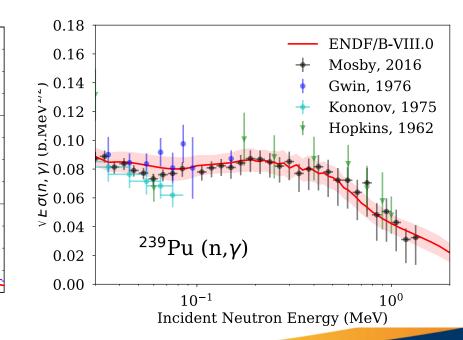






- New experimental results from DANCE measurement (Mosby et al.)
- New theoretical work (Kawano, CoH<sub>3</sub>), including M1 "scissors" mode (also, Ullmann et al.)



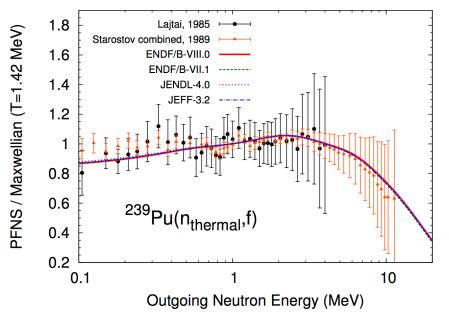


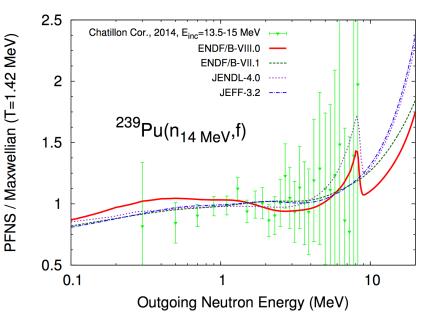




### **Prompt Fission Neutron Spectrum**

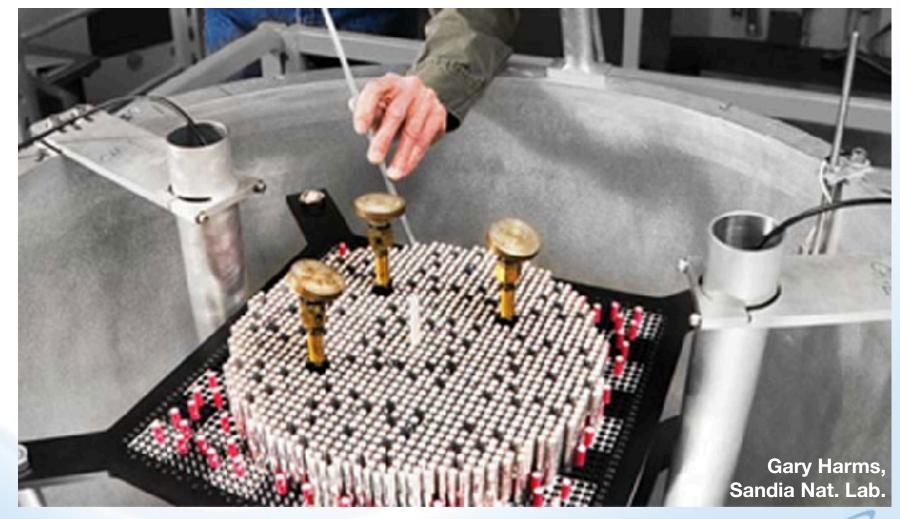
- Small tweak for thermal PFNS to improve modeling of Plutonium thermal solution benchmarks
- Unchanged from B-VII.1 from 0.5 to 5 MeV
- New evaluation (Neudecker et al.) above 5 MeV
- Preliminary chi-nu data (Kelly et al.)





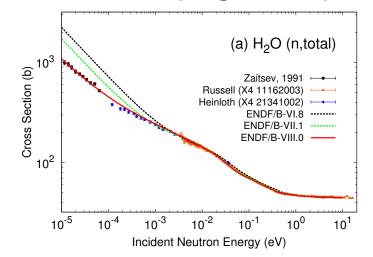
# Light water used in LWR, PWR, many solution assemblies





# Light water re-evaluated by Centro Atomico Bariloche (Argentina)





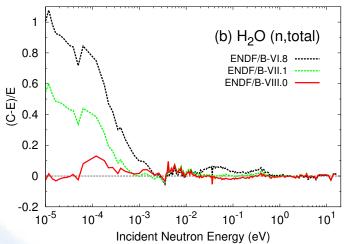


FIG. 125. (Color online) Evaluated <sup>1</sup>H<sub>2</sub>O(n,tot) total cross section at 293.6 K, compared with data retrieved from EXFOR and published by Zaitsev *et al.* [338].

- CAB Light water model
- Molecular diffusion using a modified Egelstaff-Schofield diffusion model.
- A continuous spectrum derived from molecular dynamics simulations
- Alpha and beta grids were refined

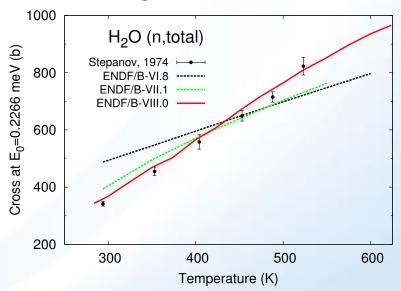
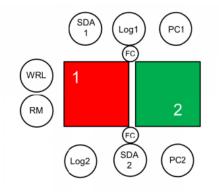


FIG. 126. (Color online) Evaluated  ${}^{1}\text{H}_{2}\text{O}(\text{n,tot})$  total cross section at different temperatures, compared with data measured by Stepanov *et al.* [339, 340] at 0.2266 meV.

### Neptune Experiment Used for Validation of ENDF/B-VIII.0(β5) H-H<sub>2</sub>O TSL as a Function of Temperature

- Rolls-Royce conducted a series of critical experiments at the Neptune facility to validate the ability to predict criticality for water-isolated arrays as function of temperature [see Ref.].
- Configurations were neutronically similar to spent fuel storage racks without poison inserts in flux trap.
- Test was specifically designed to assess criticality safety issues for spent fuel rack configurations with water gaps.
- In this configuration, undermoderated fuel assemblies can have a positive temperature coefficient of reactivity.
- Water temperature varied from 20-60 °C

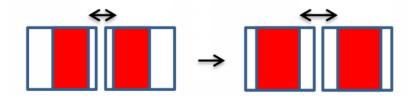
#### **Schematic of Core and Detector Arrangement**



FC = Fission Chamber SDA = ShutDown Amplifier Log = Log Channel PC = Pulse Channel

WRL = Wide Range Linear RM = Reactivity Meter

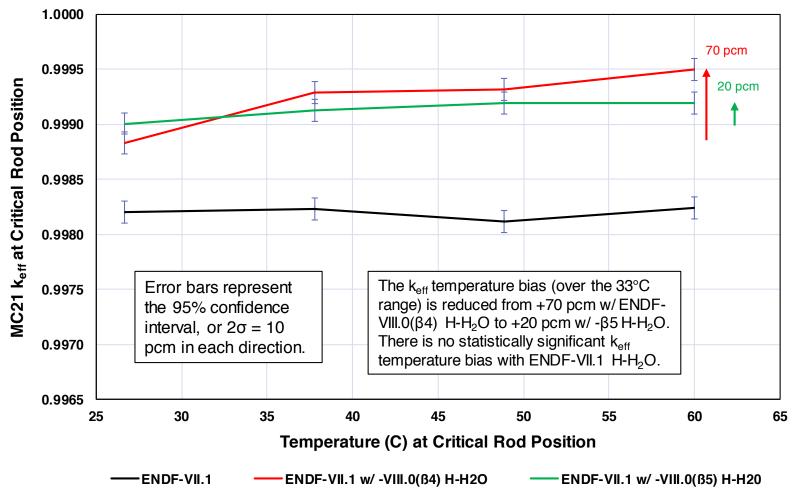
Schematic of Fuel Arrangement Showing Increase in Effective Water Gap



Ref.: S. Walley et al., "Measurement of Positive Temperature Coefficients of Reactivity for Rack-like Arrangements of Reactor Fuel in the Neptune Zero Energy Facility," Proc. RRFM-2016, Berlin, March 13-17, 2016.



# MC21 Calculated k<sub>eff</sub> for Neptune Configuration C as a Function of Temperature Using ENDF/B-VII.1 Non-Moderator Libraries and Various H-H<sub>2</sub>O TSL Libraries





# Outline for remainder of talk



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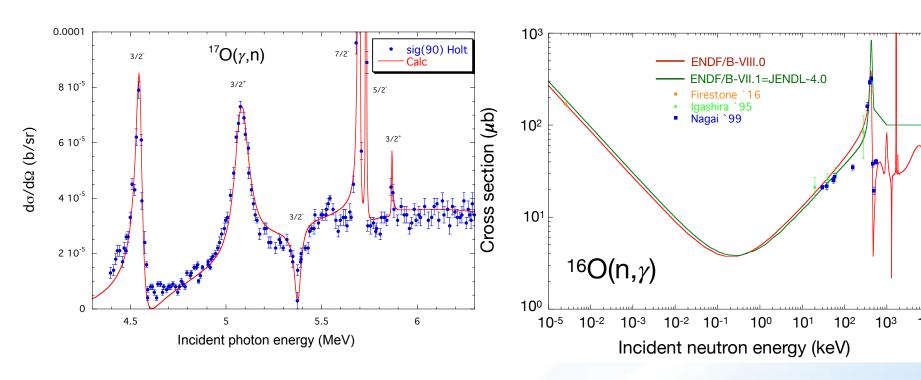
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### <sup>16</sup>O is product of R-matrix evaluation from LANL for CIELO



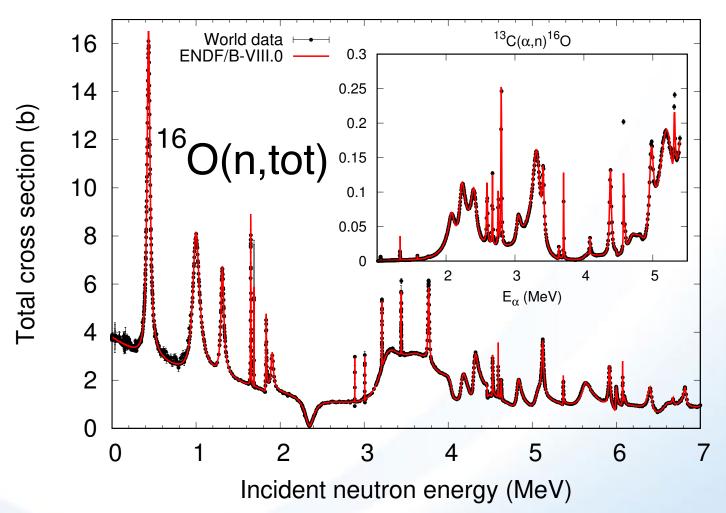


# Must consider all channels that connect to <sup>17</sup>O compound nucleus

D. Brown et al., Nuclear Data Sheets 418, 1 (2018)







D. Brown et al., Nuclear Data Sheets 418, 1 (2018)

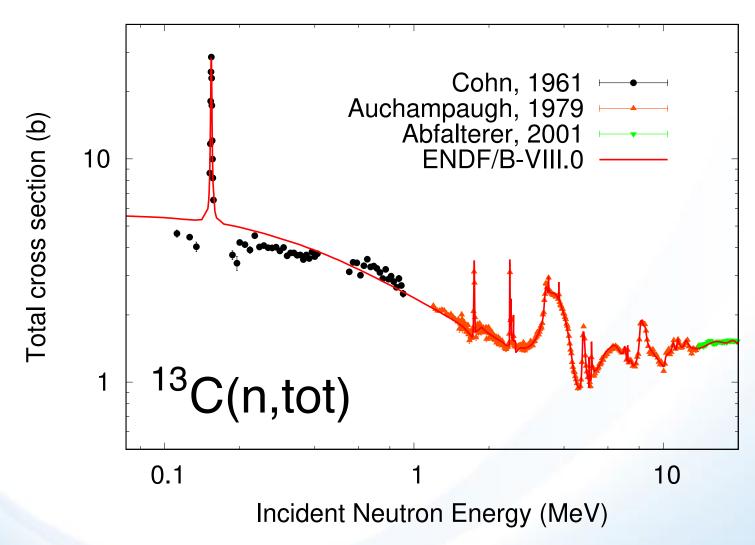


# Consideration of $^{16}O(n,\alpha)$ requires consideration of $^{13}C(\alpha,n)$ and therefore C standards



60%	р	р	р	EC	EC	100	β-	β-
2	013	014	015	016	017	<b>O18</b>	019	O20
eV	8.58 ms (3/2-)	70.606 s 0+	122.24 s 1/2-	<b>/</b> }÷ = =	- 5/2+	0+	26.91 s 5/2+	13.51
	` ′	EC	EC				β-	β-
	ECp			9.762	<b>0.038</b>	0.200		
L.	N12	N13	N14	N15	N16	N17	N18	N19
$\mathbf{v}$	11.000 ms	9.965 m	4.		7.13 s	4.173 s	624 ms	0.304
	1+	1/2-	1+	1/2-	2-	1/2-	1-	(1/2-)
	ΕC3α	EC	99.634	0.366	β-α	β-n	β-n,β-α,	β-n
)	C11	C12	C13	C14	C15	C16	C17	C18
S	20.39 m			5730 y	2.449 s	0.747 s	193 ms	95 ms
	3/2-	0+	1/	0+	1/2+	0+		0+
	EC	98.90	1.10	β-	β-	β∗ <b>n</b>	β·n	β·n
	B10	ВШ	B12	B13	B14	B15	B16	B17
${ m eV}$			20.20 ms	17.36 ms	13.8 ms	10.5 ms	200 Ps	5.08 m
	3+	3/2-	1+	3/2-	2-		(0-)	(3/2-)
	19.9	80.1	β-3α	β·n	β-	β-	n	β·n
	Be9	Be10	Be11	Be12	Be13	Be14		
7		1.51E+6 v	13.81 s	23.6 ms	0.9 MeV	4.35 ms		1/



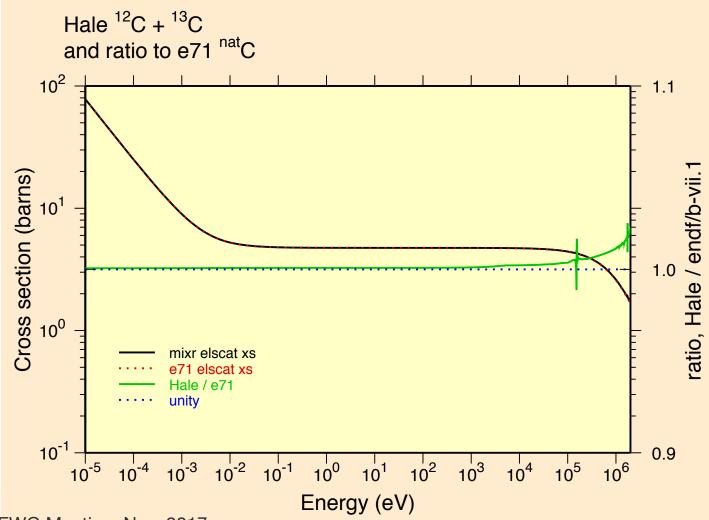


D. Brown et al., Nuclear Data Sheets 418, 1 (2018)



# Elastic cross section for natural Carbon is a Standard



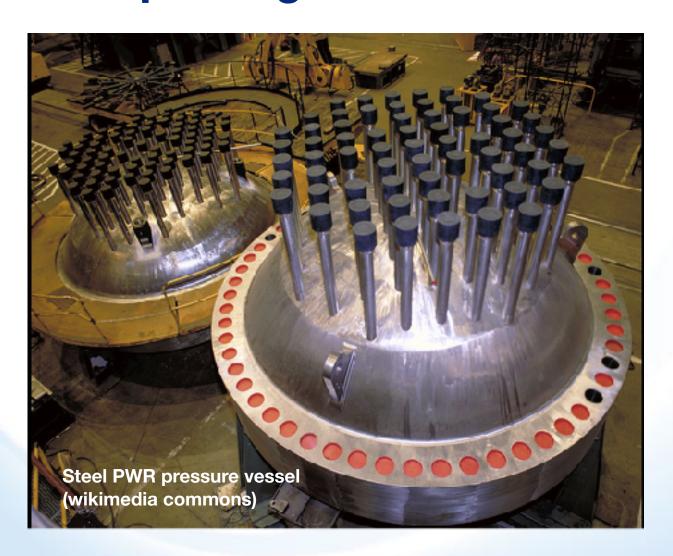


G. Hale CSEWG Meeting, Nov. 2017

BHUUKHAVEN NATIONAL LABORATORY

# New <sup>56</sup>Fe evaluation really aimed at improving steel





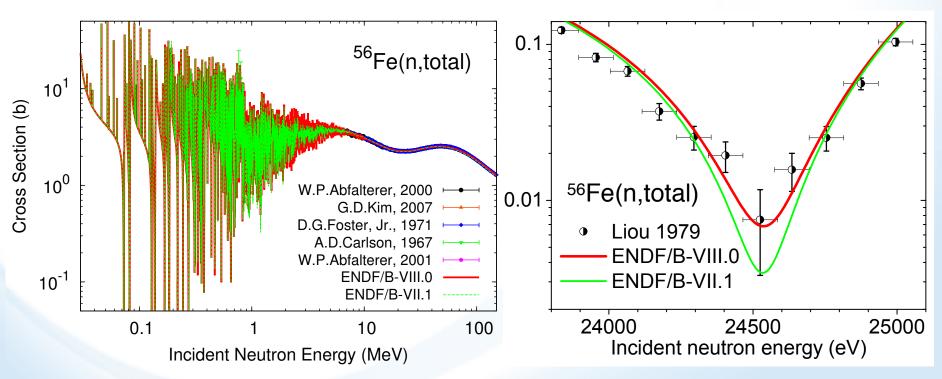
- <sup>56</sup>Fe(CIELO)
- 54,57,58**Fe**
- 59Co
- 58-62,64**N**j
- 12,13C(NeutronDataStandards)





### Resonances in <sup>56</sup>Fe go back to Froehner

- Minor correction to the previous evaluations
- Fluctuations extend high in energy





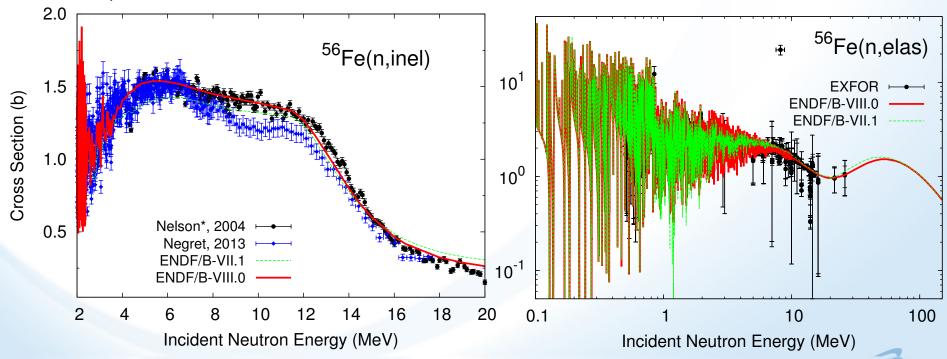


### Elastic & inelastic for 56Fe



Fluctuations imposed on inelastic scattering to the first and second excited states taken from experimental data

Elastic obtained by subtracting the sum of all reactions from the total

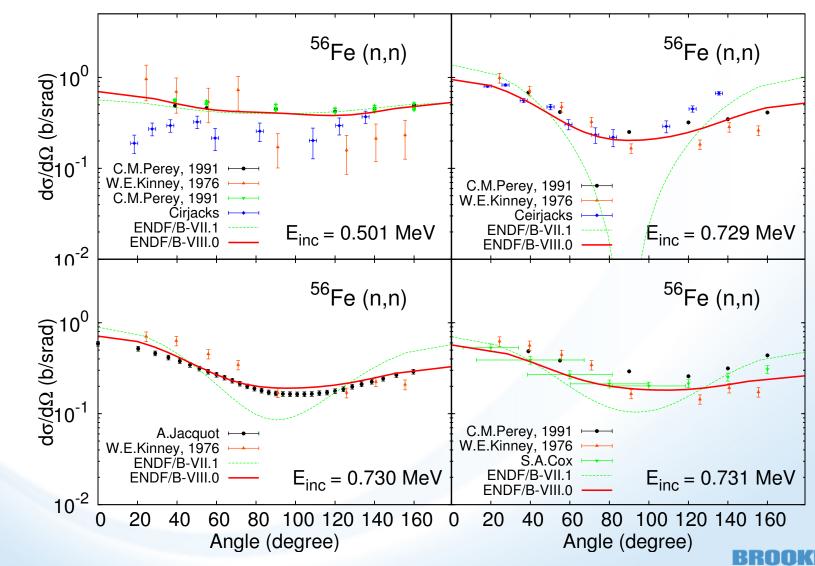


M. Herman et al., CIELO meeting, IAEA, Vienna -Dec 16-22, 2017

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### Elastic angular distributions

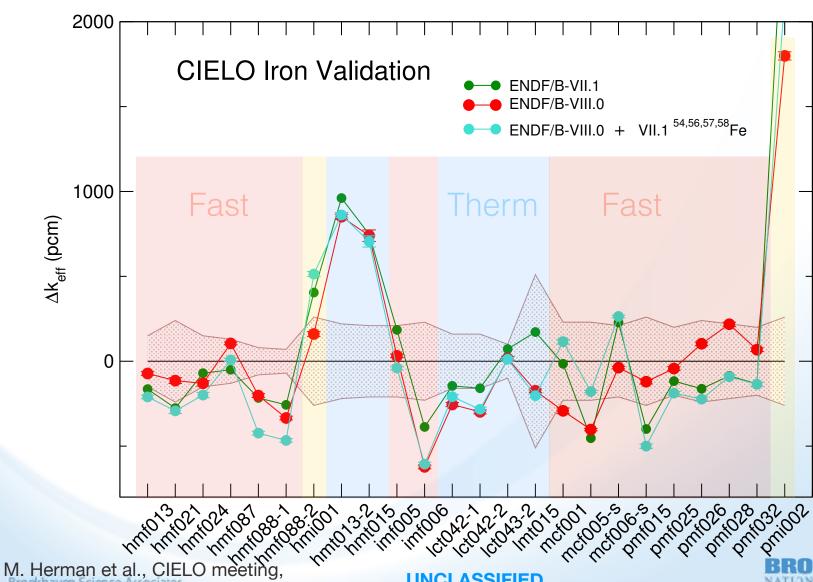




### Validation in critical assemblies

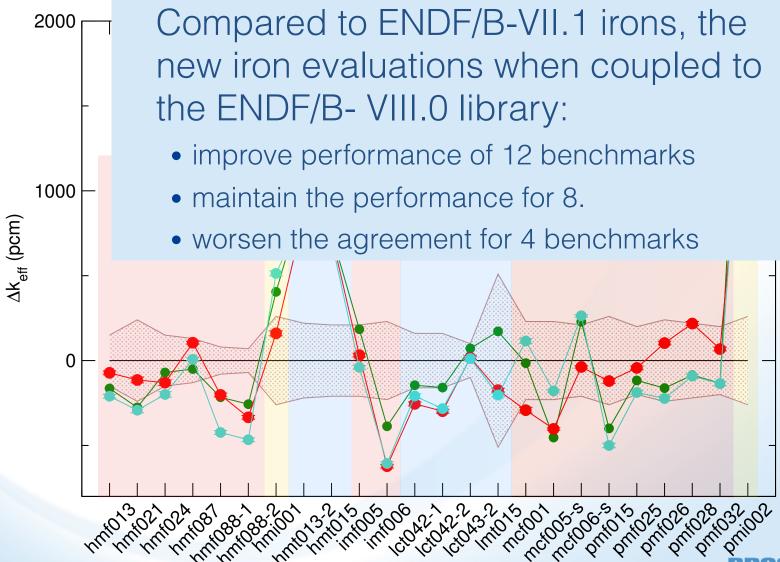
IAEA, Vienna -Dec 16-22, 2017





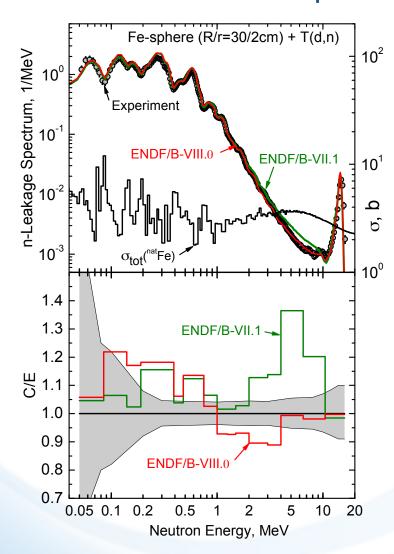
### Validation in critical assemblies

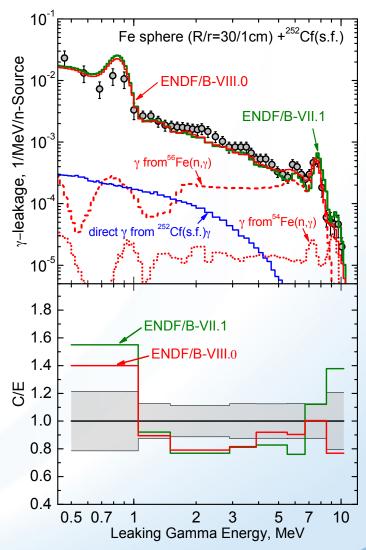




# Validation - better results in some transmission experiments





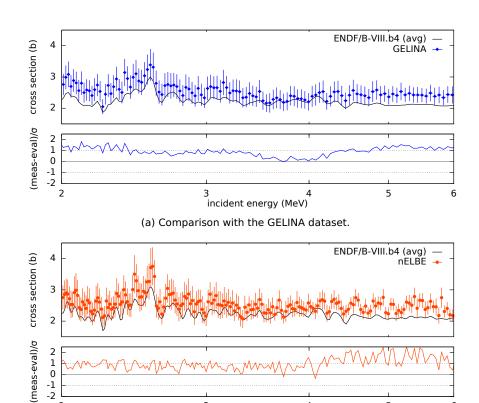


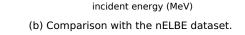
M. Herman et al., CIELO meeting, IAEA, Vienna -Dec 16-22, 2017

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### ...but worse in some others







Neutron scattering

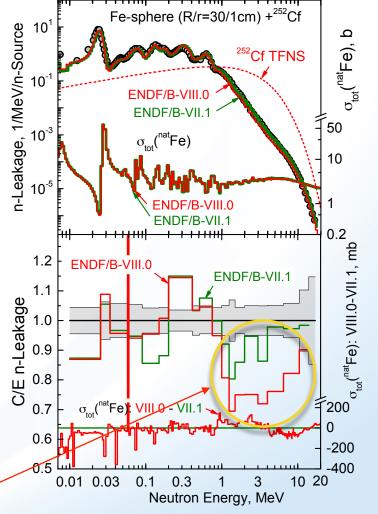
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UNIVERSITEIT

cross section measurements with a new scintillator array Elisa Pirovano

Our elastic is too low or not enough forward peaked!



M. Herman et al., CIELO meeting, IAEA, Vienna -Dec 16-22, 2017

**UNCLASSIFIED** 



# TREAT reactor@INL restarted Nov 14, 2017: need graphite





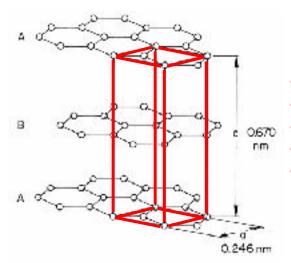
- Graphite moderated
- Materials testing
- Shut down in 1994
- After
   Fukushima,
   interest in
   restarting

TREAT Reactor (wikimedia commons)



# Graphite

Ideal "crystalline" graphite consists of planes (sheets) of carbon atoms arranged in a hexagonal lattice. Covalent bonding exits between intraplaner atoms, while the interplaner bonding is of the weak Van der Waals type. The planes are stacked in an "abab" sequence.



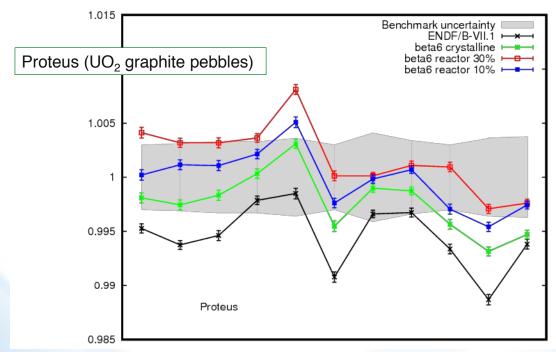
- Hexagonal Structure
- 4 atoms per unit cell
- a = b = 2.46 Å
- c = 6.7 Å
- Density = 2.25 g/cm<sup>3</sup>

Reactor graphite consists of ideal graphite crystallites (randomly oriented) in a carbon binder. It is highly porous structure with porosity level ranging between 10% and 30%.

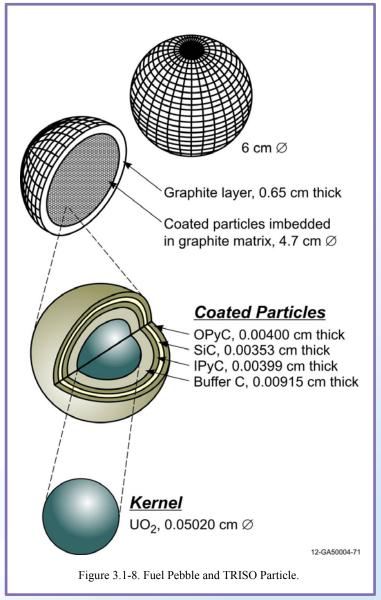


Nuclear Graphite (SEM at NCSU) Density =  $1.5 - 1.8 \text{ g/cm}^3$ 

# PROTEUS reactor is cleanest test case for graphite



Calculation curtesy of S. Van der Marck



J.D. Bess, et al. NEA/NSC/DOC(2006)1

BROOKHAVEN NATIONAL LABORATORY

### Main message



- ENDF/B-VII.1 was very good
  - k<sub>eff</sub>=1 is "baked in", which surprisingly is a problem for many customers
  - k<sub>eff</sub>=1 but with really big uncertainty does mean we biased the mean somehow, but were conservative with our uncertainty estimates
- ENDF/B-VII.1 was good, but ENDF/B-VIII.0 is much better
- There is still a lot of room for improvement
- Files available at <a href="http://www.nndc.bnl.gov/endf/b8.0/">http://www.nndc.bnl.gov/endf/b8.0/</a> download.html



# Happy 50 ± 1 Anniversary!\*

\* CSEWG formed in 1966 ENDF/B-I released in 1968

